An Approach to Quantitative Interpretation of XRD Patterns of Mineral Mixtures Using Standard Reference Minerals and Their FWHM in the PXRD-Whole Rock Difractograms

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In this experimental study composite mineral mixture composed of montmorillonite (SAz-1), quartz, calcite, and dolomite mineral standards and reference minerals was analysed. Each of 40 samples prepared as consist of 25 % (by weight) montmorillonite, quartz, calcite and dolomite was analysed.

For XRD whole rock analysis (bulk mineralogy), powdered and oriented samples were prepared via the "home method" Conditions for XRD were the following; generator: Rigaku D/Max-2200 Ultima+/PC, tube: Cu Kα=1.54059 Å, filter: Ni, accelerating voltage: 40kV, current: 20mA, goniometer speed: 1^{o}/min, and range: 2-60^{o} 2 theta. The XRD instrument were calibrated using silicon powder (NIST SRM 640-c) before its use, and minerals identified using International Center for Diffraction Data-Inorganic Crystal Structure Database (PDF-2).

FWHM values of 001 reflections of montmorillonite, quartz, calcite and dolomite minerals in whole rock diffractograms obtained from 40 separate XRD-whole rock analysis have been measured. Relative response ratios of the other whole rock mineral components with respect to quartz have been calculated by using the average FWHM referans value by the use of averages of FWHM and relative response ratios values have been calculated as 1, 1/5,36, 1/1,26 and 1/1,72 for quartz, montmorillonite, calcite and dolomite, respectively. Relative response ratios values were used in the $W_i = (K_i.FWHM_i / \Sigma K_i.FWHM_i)X100$ formula to obtain the relative abundances by weight and then the averages of these calculated relative abundance values were obtained. Standart deviation numbers of the calculated relative abundance values are less than % 2 and 1,33, 0,82, 0,98 and 0,70 were obtained for montmorillonite, quartz, calcite, and dolomite, respectively. When the known and found relative abundance values are compared and it is concluded that this analytic approach compares favorably with the other quantitative analysis techniques.

The laboratories at the Turkish Petroleum Corporation (TPAO) now have adequate equipment and trained personnel that can handle the semi-quantitative analyses of minerals and act as a referee laboratory in Turkey.